

Heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoro-
1546-95-8 | DTXSID70165670

Model Performance

Model

Data

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.91 | 1.08 | 0.91 | 1.08 | 0.92 | 1.00 |

Model Results

Predicted value: 1.03e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.13e-01

Confidence level: 2.53e-01

Nearest Neighbors from the Training Set

| | | |
|--|--|--|
| <div>Image not found</div> <div>2-Butene, 1,1,1,2,3,4,4,4-octafluoro-</div> <div>Measured: 1.33e-01</div> <div>Predicted: 2800</div> | <div>Image not found</div> <div>1,2-Dichloro-4-(trifluoromethyl)benzene</div> <div>Measured: 5.25e-01</div> <div>Predicted: 2.42</div> | <div>Image not found</div> <div>1-Butanol, 2,2,3,3,4,4,4-heptafluoro-</div> <div>Measured: 6.37</div> <div>Predicted: 42.6</div> |
| <div>Image not found</div> <div>Benazolin</div> <div>Measured: 4.28e-07</div> <div>Predicted: 8.30e-09</div> | <div>Image not found</div> <div>Silane, chlorodimethylphenyl-</div> <div>Measured: 2.91</div> <div>Predicted: 1.01</div> | |